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(FILE 'HOME' ENTERED AT 08:47:24 ON 09 FEB 2005)

FILE 'HCAPLUS' ENTERED AT 08:47:32 ON 09 FEB 2005

E EP1999-114649/AP,PRN
L1 1 EP1999-114649/AP,PRN
E W02000-EP6769/SP,PRN
E W02000-EP6769/AP,PRN
L2 1 W02000-EP6769/AP,PRN
L3 1 L1-2

FILE 'REGISTRY' ENTERED AT 08:48:53 ON 09 FEB 2005

FILE 'HCAPLUS' ENTERED AT 08:48:54 ON 09 FEB 2005
L4 TRA L3 1- RN : 83 TERMS

FILE 'REGISTRY' ENTERED AT 08:48:55 ON 09 FEB 2005
L5 83 SEA L4

FILE 'WPIX' ENTERED AT 08:48:58 ON 09 FEB 2005

E EP1999-114649/AP,PRN
L6 1 EP1999-114649/AP,PRN
E W02000-EP6769/SP,PRN
E W02000-EP6769/AP,PRN
L7 1 W02000-EP6769/AP,PRN
L8 1 L6-7

=> b hcap

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FILE COVERS 1907 - 9 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 8 Feb 2005 (20050208/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all 13

L3 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:78409 HCAPLUS
DN 134:131818
ED Entered STN: 02 Feb 2001
TI Preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents
IN Bansi, Lal; Vitthal, Genbhau Gund; Ashok, Kumar Gangopadhyay
PA Aventis Pharma Deutschland G.m.b.H., Germany
SO PCT Int. Appl.. 67 pp.
CODEN: PIXXD2

APP

DT Patent
 LA English
 IC ICM C07K007-56
 ICS A61K038-12; A61P031-10
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1

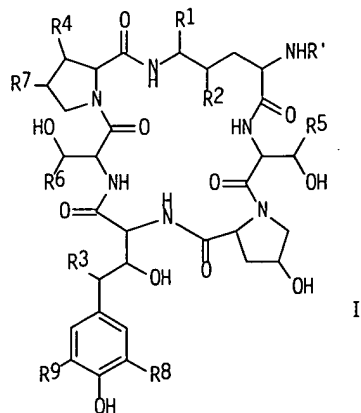
FAN.CNT 1

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PI	WO 2001007468	A2	20010201	WO 2000-EP6769	20000715 <--
	WO 2001007468	A3	20011108		
	W:	AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	CA 2380176	AA	20010201	CA 2000-2380176	20000715 <--
	EP 1204677	A2	20020515	EP 2000-953050	20000715 <--
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
	JP 2003505468	T2	20030212	JP 2001-512551	20000715 <--
PRAI	EP 1999-114649	A	19990727	<--	
	WO 2000-EP6769	W	20000715	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001007468	ICM	C07K007-56
	ICS	A61K038-12; A61P031-10

OS CASREACT 134:131818; MARPAT 134:131818
 GI



AB Cyclohexapeptides I [R' = alkyl, alkenyl, Ph, biphenyl, terphenyl, naphthyl, alkyl-, alkenyl-, or alkoxyphenyl, linoleoyl, palmitoyl, 12-methylmyristoyl, 10,12-dimethylmyristoyl, or COC6H4OC8H17-p; R1, R3 = OH, CN, CH2NH2, N3, (un)substituted aryl or heterocyclyl with 1-3 of the same or different heteroatoms, aminoalkylamino, (un)substituted alkoxy, etc.; R2, R4 = H, OH; R5 = H, Me; R6 = H, Me, CH2CONH2; R7 = H, Me, OH; R8, R9 = H or secondary aminomethyl] or their pharmaceutically acceptable salts were prepared for use as antifungal agents. Thus, mulundocandin underwent mono- and dibenzoylation on treatment with benzy] alc. and a

catalytic amount of p-toluenesulfonic acid in 1,4-dioxane.

Ornithine-5-benzylmulundocandin underwent Mannich reaction with a various secondary amines.

ST mulundocandin based cyclohexapeptide prepn antifungal; peptide cyclohexa mulundocandin based prepn antifungal

IT Fungicides

(Mannich reaction of with mulundocandin derivative)

IT Peptides, preparation

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);

USES (Uses)

(cyclic; Mannich reaction of with mulundocandin derivative)

IT 92-54-6, 1-Phenylpiperazine 102-97-6, n-Isopropylbenzylamine 103-49-1.

Dibenzylamine 123-75-1, Pyrrolidine, reactions 288-32-4, Imidazole,

reactions 626-58-4, 4-Methylpiperidine 1008-91-9, 1-(4-

Pyridyl)piperazine 1011-15-0, 1-(2-Fluorophenyl)piperazine 1012-91-5,

1-(2,6-Dimethylphenyl)piperazine 2252-63-3 2759-28-6,

1-Benzylpiperazine 3378-72-1, n-tert-Butylbenzylamine 4897-50-1,

4-Piperidinopiperidine 15532-75-9 20980-22-7 34803-66-2,

1-(2-Pyridyl)piperazine 39512-50-0, 1-(2-Chlorophenyl)piperazine

39593-08-3, 1-(4-Methylphenyl)piperazine 69628-75-7,

1-(1-Phenylethyl)piperazine

RL: RCT (Reactant); RACT (Reactant or reagent)

(Mannich reaction with mulundocandin derivative)

IT 110-89-4, Piperidine, reactions 2365-48-2, Methyl thioglycolate

108351-20-8, Mulundocandin

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)

IT 321660-96-2P 321660-97-3P 321661-50-1P 321745-36-2P 321745-66-8P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);

USES (Uses)

(preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)

IT 321660-98-4P 321660-99-5P 321661-01-2P 321661-04-5P 321661-05-6P

321661-06-7P 321661-07-8P 321661-09-0P 321661-11-4P 321661-13-6P

321661-15-8P 321661-17-0P 321661-19-2P 321661-20-5P 321661-21-6P

321661-22-7P 321661-23-8P 321661-24-9P 321661-25-0P 321661-26-1P

321661-28-3P 321661-30-7P 321661-31-8P 321661-32-9P 321661-33-0P

321661-34-1P 321661-43-2P 321661-44-3P 321661-45-4P 321661-46-5P

321661-48-7P 321661-49-8P 321661-52-3P 321661-54-5P 321661-55-6P

321661-56-7P 321661-57-8P 321745-38-4P 321745-40-8P 321745-42-0P

321745-44-2P 321745-46-4P 321745-48-6P 321745-50-0P 321745-52-2P

321745-54-4P 321745-56-6P 321745-58-8P 321745-60-2P 321745-62-4P

321745-64-6P 321745-68-0P 321745-70-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

study); PREP (Preparation); USES (Uses)

(preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)

IT 108-98-5, Thiophenol, reactions 2038-03-1, 4-(2-Aminoethyl)morpholine

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with mulundocandin derivative)

IT 321661-58-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction; preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)

=> b wpix

FILE 'WPIX' ENTERED AT 08:50:15 ON 09 FEB 2005

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FILE LAST UPDATED: 7 FEB 2005 <20050207/UP>

Search done by Noble Jarrell

MOST RECENT DERWENT UPDATE: 200509 <200509/Dw>
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 FOR DETAILS. <<<

=> d all 18

L8 ANSWER 1 OF 1 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
 AN 2001-168536 [17] WPIX
 DNC C2001-050357
 TI New cyclohexapeptide compounds useful as antifungal agents for the
 treatment of mycotic infections caused by e.g. Candida or Aspergillus.
 DC B02 B04 C02
 IN ASHOK, K G; BANSI, L; VITTHAL, G G
 PA (AVET) AVENTIS PHARMA DEUT GMBH
 CYC 86
 PI WO 2001007468 A2 20010201 (200117)* EN 67 C07K007-56
 RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
 NL OA PT SD SE SL SZ TZ UG ZW
 W: AE AG AL AU BA BB BG BR BZ CA CN CR CU CZ DM DZ EE GD GE HR HU ID
 IL IN IS JP KP KR LC LK LR LT LV MA MG MK MN MX NO NZ PL RO SG SI
 SK TR TT UA US UZ VN YU ZA
 AU 2000065640 A 20010213 (200128) C07K007-56
 EP 1204677 A2 20020515 (200239) EN C07K007-56
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 RO SE SI
 JP 2003505468 W 20030212 (200321) 92 C07K007-56
 ADT WO 2001007468 A2 WO 2000-EP6769 20000715; AU 2000065640 A AU
 2000-65640 20000715; EP 1204677 A2 EP 2000-953050 20000715, WO
 2000-EP6769 20000715; JP 2003505468 W WO 2000-EP6769 20000715
 , JP 2001-512551 20000715
 FDT AU 2000065640 A Based on WO 2001007468; EP 1204677 A2 Based on WO
 2001007468; JP 2003505468 W Based on WO 2001007468
 PRAI EP 1999-114649 19990727
 IC ICM C07K007-56
 ICS A61K038-00; A61K038-12; A61P031-04; A61P031-10
 AB WO 200107468 A UPAB: 20010328
 NOVELTY - Cyclohexapeptide compounds (I), useful as antifungal agents for
 the treatment of mycotic infections are new.

APP

DETAILED DESCRIPTION - Cyclohexapeptide compounds of formula (I), useful as antifungal agents for the treatment of mycotic infections are new.

R' = 1-20C alkyl, 9-20C alkenyl, 9-20C alkoxyphenyl, an aryl selected from phenyl, biphenyl, terphenyl and naphthyl, 1-12C alkylphenyl, 2-12C alkenylphenyl, 1-12C alkoxyphenyl, linoleoyl, palmitoyl, 12-methylmyristoyl, 10,12-dimethylmyristoyl, or -COC6H4(p)OC8H17;

R1 = -OH, -CN, -CH2NH2, -N3, aryl, substituted aryl, heterocyclic substituted heterocyclic with 1-3 heteroatoms, aminoalkylamino, mono- or di-substituted linear or cyclic aminoalkylamino, -OR; or

R = 1-12C alkyl, substituted alkyl of the type (CH2)n-X;
n = 1-5;

X = Cl, Br, I, COOY, CN, NH2 or a heterocyclic;

Y = 1-6C alkyl, 2-12C-alkenyl, aryl, fused aryl, substituted aryl, a heterocyclic containing 1-3 heteroatoms, mono or di-substituted aminoalkyl, or a hydroxy protecting group;

R3 = R1 or imidazolyl;

R2, R4 = H or OH;

R5 = H or Me;

R6 = H, Me or CH2CONH2;

R7 = H, Me or OH; and

R8, R9 = H or CH2-secondary amine.

ACTIVITY - Fungicide; Antimycotic; Anti-HIV.

MECHANISM OF ACTION - None given.

USE - (I) are useful as anti-fungal agents (claimed). They are useful for the control of both filamentous fungi and yeast. They are especially adaptable to be used for the treatment of mycotic infections in mammals, especially those caused by Candida sp. such as C. albicans, C. tropicalis, and C. neoformans, and Aspergillus sp. such as A. fumigatus, A. flavus, and A. niger. These type of infections are usually found in immunocompromised patients such as those suffering from AIDS.

Dwg.0/0

FS CPI

FA AB; GI; DCN

MC CPI: B04-C01B; B14-A04; C04-C01B; C14-A04

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FILE 'HOME' ENTERED AT 08:50:28 ON 09 FEB 2005

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(FILE 'HOME' ENTERED AT 08:47:24 ON 09 FEB 2005)

FILE 'HCAPLUS' ENTERED AT 08:47:32 ON 09 FEB 2005

E EP1999-114649/AP.PRN
L1 1 EP1999-114649/AP.PRN
E W02000-EP6769/SP.PRN
E W02000-EP6769/AP.PRN
L2 1 W02000-EP6769/AP.PRN
L3 1 L1-2

FILE 'REGISTRY' ENTERED AT 08:48:53 ON 09 FEB 2005

FILE 'HCAPLUS' ENTERED AT 08:48:54 ON 09 FEB 2005
L4 TRA L3 1- RN : 83 TERMS

FILE 'REGISTRY' ENTERED AT 08:48:55 ON 09 FEB 2005
L5 83 SEA L4

FILE 'WPIX' ENTERED AT 08:48:58 ON 09 FEB 2005

E EP1999-114649/AP.PRN
L6 1 EP1999-114649/AP.PRN
E W02000-EP6769/SP.PRN
E W02000-EP6769/AP.PRN
L7 1 W02000-EP6769/AP.PRN
L8 1 L6-7

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L9 6 C48H77N7O16
L10 1 L9 AND MULUNDOCANDIN

FILE 'HCAPLUS' ENTERED AT 09:27:46 ON 09 FEB 2005

L11 16 L10
E LAL B/AU
L12 273 E3-9.E18-19
E GUND V/AU
L13 5 E4-5
E GANGOPADHYAY A/AU
L14 88 E3-4.E19-20
L15 526 (AVENTIS (1A) DEUTSCH?)/CS.PA
L16 4 L11 AND L12-15
L17 12 L11 NOT L16

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L18 STR
L19 0 L18
L20 STR L18
L21 0 L20
L22 7 L20 FULL
SAV TEMP L22 AUD764F0/A

FILE 'HCAPLUS' ENTERED AT 09:50:14 ON 09 FEB 2005

L23 2 L22

FILE 'REGISTRY' ENTERED AT 10:11:49 ON 09 FEB 2005

L24 STR L20
L25 0 L24
L26 5 L24 FULL
SAV TEM L26 AUD764F2/A

FILE 'HCAPLUS' ENTERED AT 10:14:17 ON 09 FEB 2005

L27 2 L26
L28 2 L23 OR L27

L29

0 L12-15 AND L28

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DICTIONARY FILE UPDATES: 7 FEB 2005 HIGHEST RN 827299-31-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

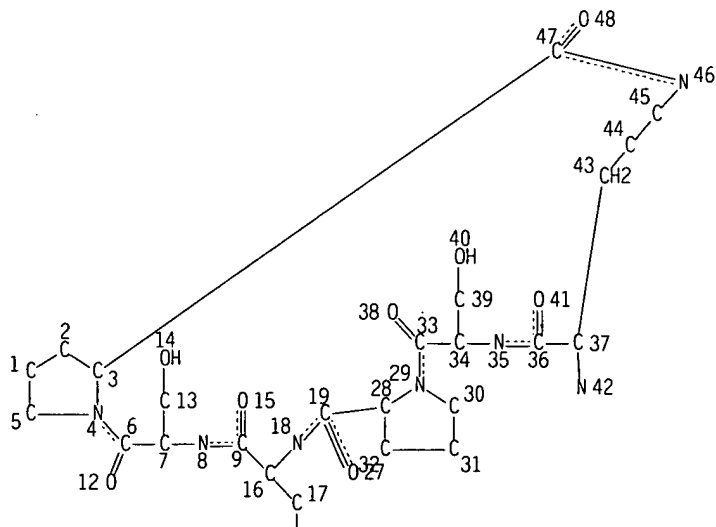
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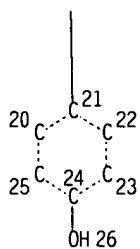
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L20 STR



Page 1-A



Page 2-A

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 DEFAULT ECLEVEL IS LIMITED

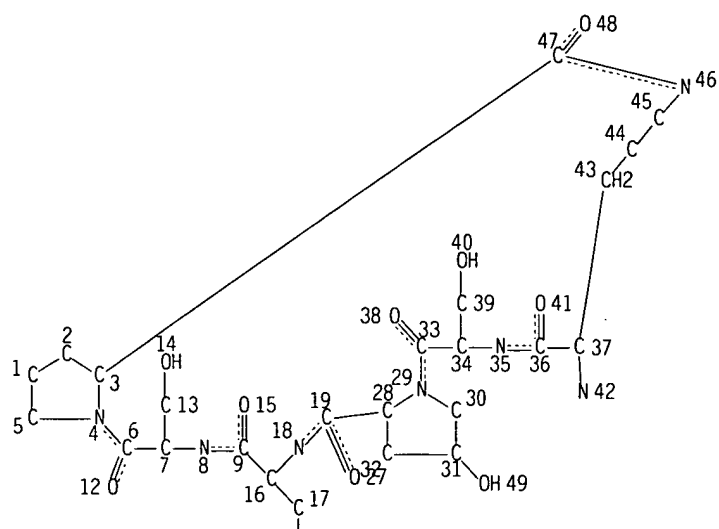
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STEREO ATTRIBUTES: NONE
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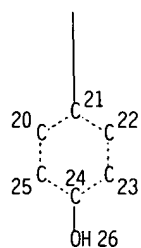
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7 ANSWERS

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 L24 STR



Page 1-A



Page 2-A

NODE ATTRIBUTES:
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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC 21
 NUMBER OF NODES IS 47

STEREO ATTRIBUTES: NONE
 L26 5 SEA FILE=REGISTRY SSS FUL L24

100.0% PROCESSED 201 ITERATIONS
SEARCH TIME: 00.00.01

5 ANSWERS

=> d ide l10 tot

L10 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN

RN 108351-20-8 REGISTRY

CN Mulundocandin (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-Dipyrrolo[2,1-c:2'.1'-1][1,4,7,10,13,16]hexaazacyclohepticosine, cyclic peptide deriv.

CN Echinocandin B, 1-[4,5-dihydroxy-N2-(12-methyl-1-oxotetradecyl)ornithine]-5-serine-

OTHER NAMES:

CN L-Proline, (4R,5R)-4,5-dihydroxy-N2-(12-methyl-1-oxotetradecyl)-L-ornithyl-L-threonyl-trans-4-hydroxy-L-prolyl-(S)-4-hydroxy-4-(4-hydroxyphenyl)-L-threonyl-L-seryl-3-hydroxy-4-methyl-, cyclic (6+1)-peptide, (2 α ,3 β ,4 β)-

MF C48 H77 N7 O16

SR CA

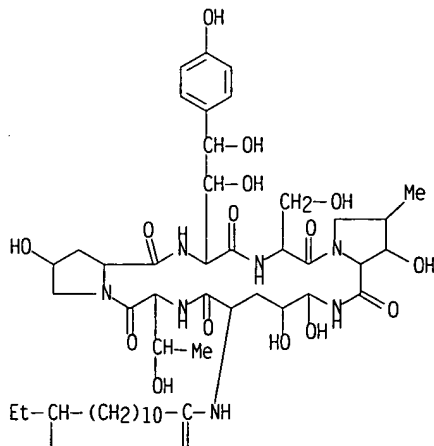
LC STN Files: BIOBUSINESS, BIOSIS, CA, CAPLUS, CASREACT, DDFU, DRUGU, MEDLINE, NAPRALERT, PHAR, PROMT, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

PAGE 1-A



PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1907 TO DATE)

Search done by Noble Jarrell

16 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> b hcap

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FILE COVERS 1907 - 9 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 8 Feb 2005 (20050208/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all fhistr l16 tot

L16 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:213956 HCAPLUS
DN 141:23332
ED Entered STN: 18 Mar 2004
TI Mannich reaction: an approach for the synthesis of water soluble mulundocandin analogues
AU Lal, Bansi; Gund, Vitthal Genbhau; Bhise, Nandu Baban; Gangopadhyay, Ashok Kumar
CS Quest Institute of LifeSciences, Nicholas Piramal India Limited, Mumbai, 4000 80, India
SO Bioorganic & Medicinal Chemistry (2004), 12(7), 1751-1768
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Ltd.
DT Journal
LA English
CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 10
OS CASREACT 141:23332
AB Semisynthetic modifications at the hydroxy tyrosine (HTyr) unit of mulundocandin were carried out to improve its aqueous solubility. Mulundocandin is a lipopeptide isolated from *Aspergillus sydowi*. A single step introduction of substituted aminomethyl groups at the ortho position(s) of phenolic hydroxyl of HTyr unit of mulundocandin has been achieved in 7-85% yield. The in vitro screening of Mannich products against *Candida albicans* and *Aspergillus fumigatus*, retained the in vivo activity of parent by oral and i.p. route. One compound showed significant improvement in activity over mulundocandin and activity compares well with that of fluconazole.
ST mulundocandin prepn aq soly Mannich reaction aminomethylation; echinocandin mulundocandin prepn aq soly Mannich reaction aminomethylation; fungicide mulundocandin prepn aq soly Mannich reaction aminomethylation; antifungal mulundocandin prepn aq soly Mannich reaction aminomethylation; *Candida* mulundocandin prepn aq soly Mannich reaction aminomethylation; *Aspergillus* mulundocandin prepn aq soly Mannich reaction aminomethylation

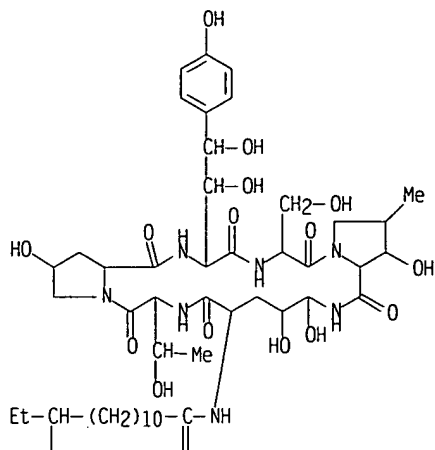
- IT Mannich bases
 RL: PAC (Pharmacological activity): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation)
 (mulundocandin derivs.: preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)
- IT Fungicides
 Mannich reaction
 Solubility
 (preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)
- IT Amines, reactions
 RL: RCT (Reactant): RACT (Reactant or reagent)
 (secondary: preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)
- IT 321660-99-5P 321661-15-8P 321661-17-0P 321661-19-2P 321661-20-5P
 321661-21-6P 321661-23-8P 321661-24-9P 321661-28-3P 321661-30-7P
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 697758-53-5P
 RL: PAC (Pharmacological activity): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation)
 (preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)
- IT 92-54-6, 1-Phenylpiperazine 100-51-6, Benzenemethanol, reactions
 102-97-6, N-(1-Methylethyl)benzenemethanamine 110-89-4, Piperidine, reactions 123-75-1, Pyrrolidine, reactions 626-58-4, 4-Methylpiperidine 1008-91-9, 1-(4-Pyridinyl)piperazine 1011-15-0, 4-(2-Fluorophenyl)piperazine 2252-63-3, 1-(4-Fluorophenyl)piperazine 2759-28-6, 1-(Phenylmethyl)piperazine, 3378-72-1, N-(1,1-Dimethylethyl)benzenemethanamine 4897-50-1, 1,4'-Bipiperidine 15532-75-9, 4-[3-(Trifluoromethyl)phenyl]piperazine 20980-22-7, 2-(1-Piperazinyl)pyrimidine 34803-66-2, 1-(2-Pyridinyl)piperazine 39512-50-0 39512-51-1, 1-(2-Methylphenyl)piperazine 39593-08-3, 1-(4-Methylphenyl)piperazine 69628-75-7, 1-(1-Phenylethyl)piperazine 108351-20-8, Mulundocandin 321660-97-3
 RL: RCT (Reactant): RACT (Reactant or reagent)
 (preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)
- IT 321660-96-2P 321745-36-2P
 RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
 (preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)
- IT 321660-98-4P 321661-01-2P 321661-04-5P 321661-05-6P 321661-06-7P
 321661-07-8P 321661-11-4P 321661-13-6P 321661-22-7P 321661-25-0P
 321661-26-1P 321661-31-8P 321661-32-9P 321661-43-2P 321745-40-8P
 321745-42-0P 321745-44-2P 321745-48-6P 321745-52-2P 693827-50-8P
 693827-51-9P 693827-52-0P 693827-54-2P 697758-50-2P 697758-51-3P
 697758-52-4P
 RL: SPN (Synthetic preparation): PREP (Preparation)
 (preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)

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- IT 108351-20-8, Mulundocandin
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (preparation of water-soluble mulundocandin analogs using Mannich reaction and study of their antifungal activity)
- RN 108351-20-8 HCAPLUS
- CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L16 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:153565 HCAPLUS
 DN 140:357655
 ED Entered STN: 26 Feb 2004
 TI Approaches towards the stabilization of hemiaminal function at ornithine unit of mulundocandin
 AU Lal, Bansi; Gund, Vitthal Genbhau
 CS Quest Institute of LifeScience, Nicholas Piramal India Limited, Mumbai, Mulund, 400080, India
 SO Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1123-1128
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier Science B.V.
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1
 AB Semisynthetic modifications at position-12 (ornithine 5-position, hemiaminal function) of mulundocandin were carried out to improve its chemical stability. New carbon-carbon (C-C) and carbon-hydrogen (C-H) bonds at the hemiaminal function 12 have been introduced. Lewis acid-catalyzed introduction of an electron-rich aryl group at position-12 of mulundocandin is developed. The synthesized mulundocandin analogs were evaluated for their chemical stability and antifungal activity against *C. albicans* and *A. fumigatus*.
 ST mulundocandin analog prepn fungicide
 IT Fungicides
 (approaches towards stabilization of hemiaminal function at ornithine unit of antifungal agent mulundocandin)
 IT Peptides, preparation
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (cyclic; approaches towards stabilization of hemiaminal function at ornithine unit of antifungal agent mulundocandin)

IT 321660-96-2 321660-97-3 321661-50-1 682338-19-8
 RL: PAC (Pharmacological activity): RCT (Reactant): BIOL (Biological study): RACT (Reactant or reagent)
 (approaches towards stabilization of hemiaminal function at ornithine unit of antifungal agent mulundocandin)

IT 321661-52-3P
 RL: PAC (Pharmacological activity): RCT (Reactant): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation): RACT (Reactant or reagent)
 (approaches towards stabilization of hemiaminal function at ornithine unit of antifungal agent mulundocandin)

IT 321661-54-5P 682338-15-4P 682338-16-5P 682338-17-6P 682338-18-7P
 RL: PAC (Pharmacological activity): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation)
 (approaches towards stabilization of hemiaminal function at ornithine unit of antifungal agent mulundocandin)

IT 91-16-7, Veratrole 2365-48-2, Methyl thioglycolate 108351-20-8
 . Mulundocandin
 RL: RCT (Reactant): RACT (Reactant or reagent)
 (approaches towards stabilization of hemiaminal function at ornithine unit of antifungal agent mulundocandin)

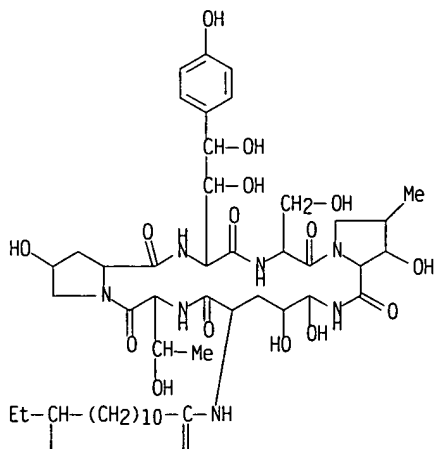
RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD

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 IT 108351-20-8, Mulundocandin
 RL: RCT (Reactant): RACT (Reactant or reagent)
 (approaches towards stabilization of hemiaminal function at ornithine unit of antifungal agent mulundocandin)
 RN 108351-20-8 HCAPLUS
 CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

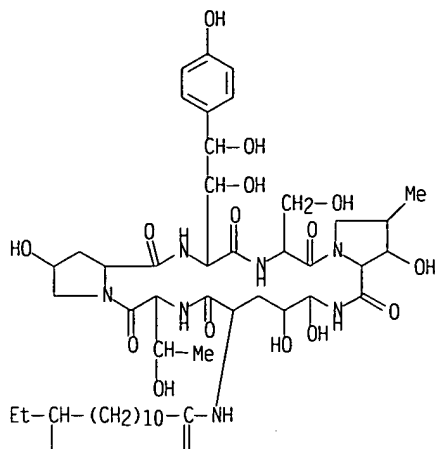


L16 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2003:867279 HCAPLUS
 DN 140:146488
 ED Entered STN: 06 Nov 2003
 TI Semisynthetic modifications of hemiaminal function at ornithine unit of mulundocandin, towards chemical stability and antifungal activity
 AU La1, Bansi; Gund, Vitthal Genbhau; Gangopadhyay,

- Ashok Kumar; Nadkarni, S. R.; Dikshit, Vidula; Chatterjee, D. K.; Shirvaikar, R.
- CS Quest Institute of LifeSciences, Department of Medicinal Chemistry, Nicholas Piramal India Limited, Mumbai, Mulund (w), 4000 80, India
- SO Bioorganic & Medicinal Chemistry (2003), 11(23), 5189-5198
CODEN: BMECEP; ISSN: 0968-0896
- PB Elsevier Ltd.
- DT Journal
- LA English
- CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
- AB Mulundocandin, is an echinocandin class of lipopeptide. It has wide spectrum of antifungal activity against Candida and Aspergillus species. Semisynthetic modification at Ornithine-5-hydroxyl (hemiaminal function) of mulundocandin was carried out to improve solution stability and hence in vivo activity. Synthesis of ether (C-OR), thioether (C-SR) and C-N linkage at hemiaminal function are described. All synthetic analogs were evaluated for their stability in aqueous solution and found to be more stable than mulundocandin. Antifungal activity of Orn-5 analogs was evaluated both in vitro against Candida albicans and Aspergillus fumigatus by agar well method and in vivo (oral and i.p.) in C. albicans infected Swiss mice. Results of in vivo assays of analogs by the oral route suggests that the introduction of either oxygen nucleophiles (-OR) or sulfur nucleophiles (-SR), at either Orn-5 or at both Orn-5 and HTyr-4 positions, results in retaining the activity of the parent compound with improved aqueous stability in most cases. I showed improved antifungal activity in comparison to mulundocandin by oral application in Swiss mice.
- ST mulundocandin analog prepn; antifungal mulundocandin analog
- IT Structure-activity relationship
(fungicidal; semisynthetic modifications of mulundocandin for the evaluation of chemical stability and antifungal activity)
- IT Fungicides
(semisynthetic modifications of mulundocandin for the evaluation of chemical stability and antifungal activity)
- IT 321661-48-7P 321745-64-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(semisynthetic modifications of mulundocandin for the evaluation of chemical stability and antifungal activity)
- IT 321660-96-2P 321660-97-3P 321661-49-8P 321661-55-6P 321661-56-7P 321661-57-8P 321745-36-2P 321745-38-4P 321745-66-8P 321745-70-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(semisynthetic modifications of mulundocandin for the evaluation of chemical stability and antifungal activity)
- IT 67-56-1, Methanol, reactions 100-51-6, Benzyl alcohol, reactions 108-98-5, Thiophenol, reactions 288-32-4, 1H-Imidazole, reactions 2038-03-1, 4-Morpholineethanamine 2365-48-2, Methylthioglycolate 108351-20-8, Mulundocandin
RL: RCT (Reactant); RACT (Reactant or reagent)
(semisynthetic modifications of mulundocandin for the evaluation of chemical stability and antifungal activity)
- IT 321661-50-1P 321661-58-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(semisynthetic modifications of mulundocandin for the evaluation of chemical stability and antifungal activity)
- RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
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- IT 108351-20-8, Mulundocandin
 RL: RCT (Reactant): RACT (Reactant or reagent)
 (semisynthetic modifications of mulundocandin for the evaluation of
 chemical stability and antifungal activity)
- RN 108351-20-8 HCAPLUS
- CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L16 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:78409 HCAPLUS
 DN 134:131818
 ED Entered STN: 02 Feb 2001
 TI Preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents
 IN Bansil, Lal; Vitthal, Genbhu Gund; Ashok, Kumar Gangopadhyay
 PA Aventis Pharma Deutschland G.m.b.H., Germany
 SO PCT Int. Appl., 67 pp.
 CODEN: PIXX02
 DT Patent
 LA English
 IC ICM C07K007-56
 ICS A61K038-12; A61P031-10
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001007468	A2	20010201	WO 2000-EP6769	20000715
	WO 2001007468	A3	20011108		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
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	EP 1204677	A2	20020515	EP 2000-953050	20000715
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APP.

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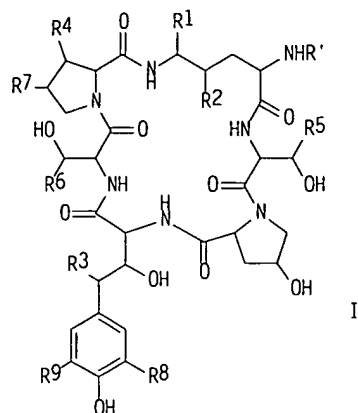
CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 2001007468 ICM C07K007-56
ICS A61K038-12; A61P031-10

OS CASREACT 134:131818; MARPAT 134:131818

GI



AB Cyclohexapeptides I [R' = alkyl, alkenyl, Ph, biphenyl, terphenyl, naphthyl, alkyl-, alkenyl-, or alkoxyphenyl, linoleoyl, palmitoyl, 12-methylmyristoyl, 10,12-dimethylmyristoyl, or COC6H4OC8H17-p; R1, R3 = OH, CN, CH2NH2, N3, (un)substituted aryl or heterocyclyl with 1-3 of the same or different heteroatoms, aminoalkylamino, (un)substituted alkoxy, etc.; R2, R4 = H, OH; R5 = H, Me; R6 = H, Me, CH2CONH2; R7 = H, Me, OH; R8, R9 = H or secondary aminomethyl] or their pharmaceutically acceptable salts were prepared for use as antifungal agents. Thus, mulundocandin underwent mono- and dibenylation on treatment with benzyl alc. and a catalytic amount of p-toluenesulfonic acid in 1,4-dioxane. Ornithine-5-benzylmulundocandin underwent Mannich reaction with a various secondary amines.

ST mulundocandin based cyclohexapeptide prepn antifungal; peptide cyclohexa mulundocandin based prepn antifungal

IT Fungicides

(Mannich reaction of with mulundocandin derivative)

IT Peptides, preparation

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(cyclic; Mannich reaction of with mulundocandin derivative)

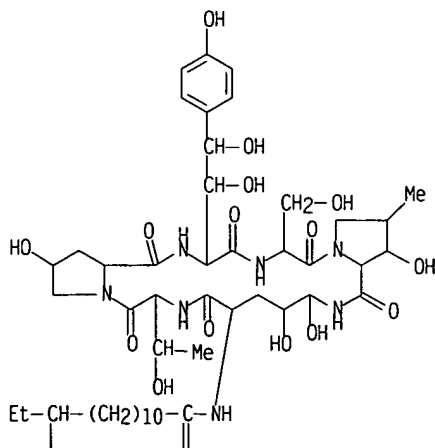
IT 92-54-6, 1-Phenylpiperazine 102-97-6, n-Isopropylbenzylamine 103-49-1, Dibenzylamine 123-75-1, Pyrrolidine, reactions 288-32-4, Imidazole, reactions 626-58-4, 4-Methylpiperidine 1008-91-9, 1-(4-Pyridyl)piperazine 1011-15-0, 1-(2-Fluorophenyl)piperazine 1012-91-5, 1-(2,6-Dimethylphenyl)piperazine 2252-63-3 2759-28-6, 1-Benzylpiperazine 3378-72-1, n-tert-Butylbenzylamine 4897-50-1, 4-Piperidinopiperidine 15532-75-9 20980-22-7 34803-66-2, 1-(2-Pyridyl)piperazine 39512-50-0, 1-(2-Chlorophenyl)piperazine 39593-08-3, 1-(4-Methylphenyl)piperazine 69628-75-7, 1-(1-Phenylethyl)piperazine

RL: RCT (Reactant); RACT (Reactant or reagent)

(Mannich reaction with mulundocandin derivative)

- IT 110-89-4. Piperidine. reactions 2365-48-2. Methyl thioglycolate
108351-20-8. Mulundocandin
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)
- IT 321660-96-2P 321660-97-3P 321661-50-1P 321745-36-2P 321745-66-8P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)
(preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)
- IT 321660-98-4P 321660-99-5P 321661-01-2P 321661-04-5P 321661-05-6P
321661-06-7P 321661-07-8P 321661-09-0P 321661-11-4P 321661-13-6P
321661-15-8P 321661-17-0P 321661-19-2P 321661-20-5P 321661-21-6P
321661-22-7P 321661-23-8P 321661-24-9P 321661-25-0P 321661-26-1P
321661-28-3P 321661-30-7P 321661-31-8P 321661-32-9P 321661-33-0P
321661-34-1P 321661-43-2P 321661-44-3P 321661-45-4P 321661-46-5P
321661-48-7P 321661-49-8P 321661-52-3P 321661-54-5P 321661-55-6P
321661-56-7P 321661-57-8P 321745-38-4P 321745-40-8P 321745-42-0P
321745-44-2P 321745-46-4P 321745-48-6P 321745-50-0P 321745-52-2P
321745-54-4P 321745-56-6P 321745-58-8P 321745-60-2P 321745-62-4P
321745-64-6P 321745-68-0P 321745-70-4P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)
- IT 108-98-5. Thiophenol. reactions 2038-03-1. 4-(2-Aminoethyl)morpholine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with mulundocandin derivative)
- IT 321661-58-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction; preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)
- IT 108351-20-8. Mulundocandin
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel cyclohexapeptides based on mulundocandin for use as antifungal agents)
- RN 108351-20-8 HCAPLUS
CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



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L17 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:244401 HCAPLUS

DN 139:49695

ED Entered STN: 30 Mar 2003

TI Drug induced proteome changes in *Candida albicans*: Comparison of the effect of $\beta(1,3)$ glucan synthase inhibitors and two triazoles, fluconazole and itraconazole

AU Bruneau, Jean-Michel; Maillet, Isabelle; Tagat, Eric; Legrand, Raymond; Supatto, Françoise; Fudali, Claude; Le Caer, Jean-Pierre; Labas, Valerie; Lecaque, Dominique; Hodgson, John

CS Infectious Disease Group, Aventis Pharma, Romainville, 93235, Fr.

SO Proteomics (2003), 3(3), 325-336

CODEN: PROTC7; ISSN: 1615-9853

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

CC 10-5 (Microbial, Algal, and Fungal Biochemistry)

AB The dimorphic fungus *C. albicans* is an opportunistic human pathogen. Candidiasis is usually treated with azole antifungal agents. However clin. treatments may fail due to the appearance of resistance to this class of antifungal agents in *Candida*. Echinocandin derivs. are an alternative for the treatment of these fungal infections and are active against azole resistant isolates of *C. albicans*. Azoles inhibit the lanosterol 14 α -demethylase, which is a key enzyme in the synthesis of ergosterol. In contrast, the echinocandin class of antibiotics inhibit noncompetitively β -(1,3)-D-glucan synthesis in vitro. We have investigated the impact of mulundocandin on the proteome of *C. albicans* and compared it to those of a mulundocandin derivative, as well as to 2 azoles of different structure, fluconazole and itraconazole. The changes in gene expression underlying the antifungal responses were analyzed by comparative 2-D PAGE. Dose dependant responses were kinetically studied on *C. albicans* grown at 25° (yeast form) in synthetic dextrose medium. This study shows that antifungals with a common mechanism of action lead to comparable effects at the proteome level and that a proteomics approach can be used to distinguish different antifungals, with the promise to become a useful tool to study drugs of unknown mechanism of action.

ST fungicide action mechanism *Candida* proteome

IT Antimicrobial agents

(action mechanism, fungicides; $\beta(1,3)$ -glucan synthase inhibitors and fluconazole and itraconazole induction of proteome changes in *Candida albicans*)

IT *Candida albicans*

Fungicides

($\beta(1,3)$ -glucan synthase inhibitors and fluconazole and itraconazole induction of proteome changes in *Candida albicans*)

IT Proteome

RL: BSU (Biological study, unclassified); BIOL (Biological study)

($\beta(1,3)$ -glucan synthase inhibitors and fluconazole and itraconazole induction of proteome changes in *Candida albicans*)

IT 84625-61-6, Itraconazole 86386-73-4, Fluconazole 108351-20-8, Mulundocandin

RL: BSU (Biological study, unclassified); BIOL (Biological study)

($\beta(1,3)$ -glucan synthase inhibitors and fluconazole and itraconazole induction of proteome changes in *Candida albicans*)

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RL: BSU (Biological study, unclassified); BIOL (Biological study)
(β (1.3)-glucan synthase inhibitors and fluconazole and
itraconazole induction of proteome changes in *Candida albicans*)

CN Mulundocandin (9CI) (CA INDEX NAME)

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PAGE 2-A

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L17 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:369771 HCAPLUS
 DN 137:180411
 ED Entered STN: 19 May 2002
 TI Development of molecular tools for the mulundocandin producer *Aspergillus sydowii*: DNA-mediated transformation and reporter gene expression
 AU Schmitt, E. K.; Eilinghoff, B.; Olliger, R.; Decker, H.; Kuck, U.
 CS Ruhr-Universität Bochum, Bochum, 44801, Germany
 SO Applied Microbiology and Biotechnology (2002), 58(5), 625-631
 CODEN: AMBIDG; ISSN: 0175-7598
 PB Springer-Verlag
 DT Journal
 LA English
 CC 3-2 (Biochemical Genetics)
 Section cross-reference(s): 10
 AB The echinocandin-type antimycotic mulundocandin and its derivs. are produced by the filamentous fungus *Aspergillus sydowii* (strain FH2551). These agents have been considered as a potential drug to treat immunocompromised patients who suffer from severe opportunistic fungal infections. In order to generate strains with a modified mulundocandin biosynthesis, we developed mol. tools for genetic engineering of *A. sydowii* as an alternative to conventional strain improvement procedures. For our expts., we used strain FH2551, which was discriminated from other *Aspergillus* strains by determining the sequence of the two internal transcribed spacers (ITS1 and ITS2) of the rDNA locus. In addition, the electrophoretic karyotype of *A. sydowii* was established using pulsed-field gel electrophoresis (PFGE), leading to a calculated genomic size of about 40 Mb. For gene mapping, chromosomes were subjected to PFGE either unrestricted or after incubation with rare cutting enzymes and probed with heterologous genes. Using the bacterial hygromycin B phosphotransferase gene as a selectable marker for transformation of *A. sydowii*, we generated transformants with single and multiple copies of plasmid DNA. Subsequently, the heterologous *lacZ* and *gfp* genes were efficiently transferred and expressed in *A. sydowii*. The majority of *lacZ*-transformants showed more than 6 pkat β -galactosidase activity/mg protein, while the control strains had no significant background activity. Fluorescence microscopy of *gfp*-transformants demonstrated that the green-fluorescent protein is present in a stable and active form in the cytoplasm of vegetative hyphae and conidiospores.
 ST *Aspergillus sydowii* electrophoretic karyotype; plasmid DNA mediated transformation *Aspergillus sydowii*; mulundocandin producer *Aspergillus*
 IT *Aspergillus sydowii*
 Transformation, genetic
 (electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)
 IT Karyotyping
 (electrophoretic, of *A. sydowii*; electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)
 IT Proteins
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (green fluorescent, reporter gene for; electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)
 IT Gene, microbial
 RL: BSU (Biological study, unclassified); BIOL (Biological study)

(hph, as selection marker; electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)

IT Gene, microbial

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(lacZ, as reporter; electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)

IT Plasmid vectors

(plasmid DNA integration into *A. sydowii* genome; electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)

IT 108351-20-8P, Mulundocandin

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)

IT 88361-67-5, Hygromycin B phosphotransferase

RL: ARU (Analytical role, unclassified); ANST (Analytical study) (selectable marker gene for; electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)

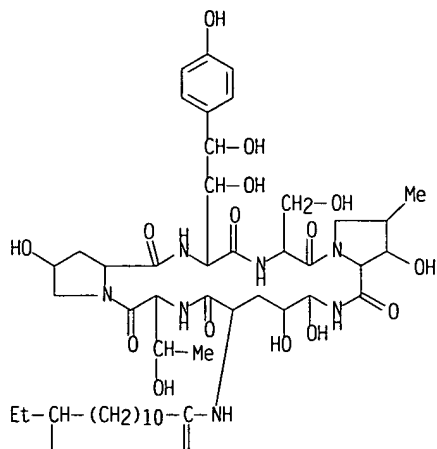
RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD

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 IT 108351-20-8P. Mulundocandin
 RL: BPN (Biosynthetic preparation): BIOL (Biological study): PREP (Preparation)
 (electrophoretic karyotype, DNA-mediated transformation and reporter gene expression for mulundocandin producer *Aspergillus sydowii*)
 RN 108351-20-8 HCAPLUS
 CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L17 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:255768 HCAPLUS
 DN 137:201573
 ED Entered STN: 05 Apr 2002
 TI Synthesis of new echinocandin derivatives via a diol-keto transposition
 AU Aszodi, Jozsef; Fauveau, Patrick; Melon-Manguer, Dominique; Ehlers, Eberhard; Schio, Laurent
 CS Medicinal Chemistry, Aventis Pharma, Romainville, F-93235, Fr.
 SO Tetrahedron Letters (2002), 43(16), 2953-2956
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 26
 OS CASREACT 137:201573
 AB A new diol-carbonyl transposition reaction has been discovered in echinocandin type structures. An α -hydroxy hemiaminal moiety has been shown to undergo a pinacol-type rearrangement in the presence of trimethylsilyl iodide to afford ketone derivs. Applied to

deoxymulundocandin. this transposition led to a useful intermediate for further chemical modification.

ST deoxymulundocandin pinacol rearrangement prepn cyclic peptide ketone

IT Peptides. preparation

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cyclic: diol-carbonyl transposition reaction of deoxymulundocandin for preparation of intermediate for further chemical modification)

IT Natural products

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(diol-carbonyl transposition reaction of deoxymulundocandin for preparation of intermediate for further chemical modification)

IT Ketones. preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(diol-carbonyl transposition reaction of deoxymulundocandin for preparation of intermediate for further chemical modification)

IT Rearrangement

(pinacol: diol-carbonyl transposition reaction of deoxymulundocandin for preparation of intermediate for further chemical modification)

IT 227472-52-8P 452916-29-9P 452916-30-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of deoxymulundocandin derivs. via diol-carbonyl transposition reaction)

IT 108351-20-8. Mulundocandin 138626-63-8. Deoxymulundocandin 227472-53-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of in the preparation of deoxymulundocandin derivs. via diol-carbonyl transposition reaction)

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT 108351-20-8. Mulundocandin

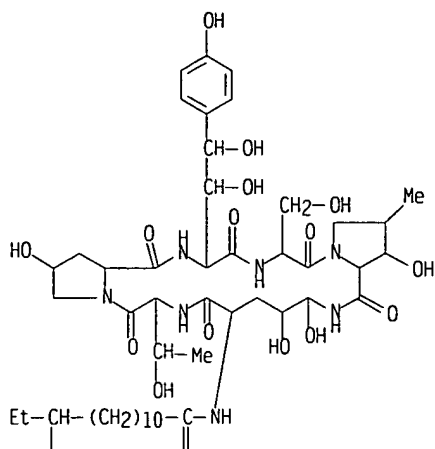
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of in the preparation of deoxymulundocandin derivs. via diol-carbonyl transposition reaction)

RN 108351-20-8 HCAPLUS

CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L17 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:618023 HCAPLUS
 DN 135:180953
 ED Entered STN: 24 Aug 2001
 TI Preparation of novel echinocandin derivatives as fungicides
 IN Courtin, Olivier; Dussarat, Arlette; Melon-Manguer, Dominique; Schio, Laurent
 PA Aventis Pharma S.A., Fr.
 SO PCT Int. Appl., 30 pp.
 CODEN: PIXXD2
 DT Patent
 LA French
 IC ICM C07K007-56
 ICS A61K038-12; A61P031-10
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1. 32

FAN.CNT 1

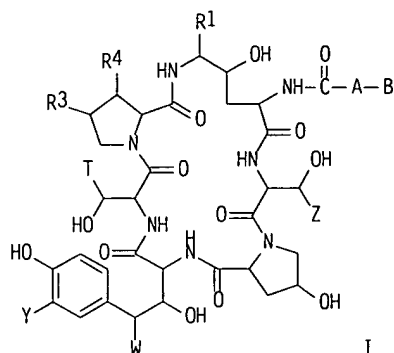
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2804957	A1	20010817	FR 2000-1844	20000215
FR 2804957	B1	20031128		
CA 2402219	AA	20010823	CA 2001-2402219	20010214
EP 1257568	A1	20021120	EP 2001-907783	20010214
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004014602	A1	20040122	US 2002-220829	20021203

PRAI FR 2000-1844 A 20000215
 WO 2001-FR419 W ~~20010214~~

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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WO 2001060845	ICM	C07K007-56
	ICS	A61K038-12: A61P031-10
FR 2804957	ECLA	C07K007/56
US 2004014602	ECLA	C07K007/56
OS MARPAT 135:180953		
GI		



AB Echinocandin derivs. I [R1 = H, OH, (un)substituted alkoxy, alkenyloxy or alkynyloxy; R3 = H, Me, OH; R4, W = H, OH; A = O, CH2, NH; B is a steroid residue; T = H, Me, CH2CONH2, CH2C.tplbond.N, (CH2)2NH2 or alkylaminoethyl; Y = H, OH, halo, OSO3H or salts; Z = H, Me] were prepared as antifungal agents. Thus, 1-[(4R,5R)-4,5-dihydroxy-N2-[[[(3β,22E)-ergosta-5,7,22-trien-3-yl]oxy]carbonyl]-L-ornithine]deoxymulundocandin was prepared by treating ergosterol with diphosgene in CH2Cl2 in the presence of Et3N and treating the product with deoxymulundocandin.

ST echinocandin steroid deriv prepn fungicide

IT Peptides, preparation

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cyclic; preparation of novel echinocandin derivs. as fungicides)

IT Fungicides

(preparation of novel echinocandin derivs. as fungicides)

IT 355127-02-5P 355127-03-6P 355127-04-7P 355127-05-8P 355127-06-9P
 355127-07-0P 355127-08-1P 355127-09-2P 355127-10-5P 355127-11-6P
 355127-12-7P 355127-13-8P 355127-14-9P 355127-15-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel echinocandin derivs. as fungicides)

IT 57-87-4, Ergosterol 57-88-5, Cholesterol, reactions 79-63-0, Lanosterol 80-97-7, 5α-Cholestan-3β-ol 83-46-5, β-Sitosterol 83-48-7, Stigmasterol 503-38-8, Diphosgene 566-88-1 5927-18-4 108351-20-8, Mulundocandin 138626-63-8, Deoxymulundocandin

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of novel echinocandin derivs. as fungicides)

IT 24698-89-3P 41238-20-4P 41238-22-6P 154005-59-1P 355127-16-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of novel echinocandin derivs. as fungicides)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Fujisawa Pharm Co Ltd: JP 05202096 A 1993 HCAPLUS

(2) Merck & Co Inc: WO 9527074 A 1995 HCAPLUS

(3) Roy, E: JOURNAL OF ANTIBIOTICS 1987. V40(3). P275

IT 108351-20-8. Mulundocandin

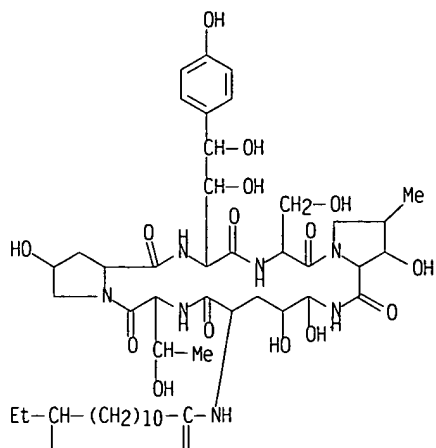
RL: RCT (Reactant): RACT (Reactant or reagent)

(preparation of novel echinocandin derivs. as fungicides)

RN 108351-20-8 HCAPLUS

CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L17 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:550050 HCAPLUS

DN 136:196475

ED Entered STN: 30 Jul 2001

TI Utility of 2,3-bis(2-methoxy-4-nitro-5-sulfophenyl)-5-[(phenyl-amino)carbonyl]-2H-tetrazolium hydroxide (XTT) and minimum effective concentration assays in the determination of antifungal susceptibility of *Aspergillus fumigatus* to the lipopeptide class of compounds

AU Hawser, S. P.; Jessup, C.; Vitullo, J.; Ghannoum, M. A.

CS Aventis, Romainville, F-93235, Fr.

SO Journal of Clinical Microbiology (2001), 39(7), 2738-2741

CODEN: JCMIDW; ISSN: 0095-1137

PB American Society for Microbiology

DT Journal

LA English

CC 9-12 (Biochemical Methods)

Section cross-reference(s): 10

AB The susceptibility of *Aspergillus fumigatus* to mulundocandin, an echinocandin-like compound, and other antifungal agents was assessed by the National Committee for Clin. Laboratory Stds. (NCCLS) M38-P method, a 2,3-bis(2-methoxy-4-nitro-5-sulfophenyl)-5-[(phenyl-amino)carbonyl]-2H-tetrazolium hydroxide (XTT)-based colorimetric assay, and determination of

morphol. alterations by microscopy. In contrast to the NCCLS M38-P method, which does not predict the activity in vivo, the XTT-based assay showed that *A. fumigatus* is susceptible to mulundocandin. Thus, the XTT-based assay might be useful for determination of the susceptibilities of molds to echinocandins.

ST XTT *Aspergillus* lipopeptide mulundocandin susceptibility

IT *Aspergillus fumigatus*

Fungicides

(utility of XTT and min. effective concentration assays in the determination of antifungal susceptibility of *Aspergillus fumigatus* to the lipopeptide class of compds.)

IT 111072-31-2. XTT

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)

(utility of XTT and min. effective concentration assays in the determination of antifungal susceptibility of *Aspergillus fumigatus* to the lipopeptide class of compds.)

IT 1397-89-3. Amphotericin B 2022-85-7. Flucytosine 84625-61-6.

Itraconazole 86386-73-4. Fluconazole 108351-20-8.

Mulundocandin

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(utility of XTT and min. effective concentration assays in the determination of antifungal susceptibility of *Aspergillus fumigatus* to the lipopeptide class of compds.)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Beaulieu, D; FEMS Microbiol Lett 1993. V108. P133 HCAPLUS

(2) Clancy, C; J Clin Microbiol 1997. V35. P2878 HCAPLUS

(3) Colombo, A; J Antimicrob Chemother 1995. V36. P93 HCAPLUS

(4) Hawser, S; J Antibiot 1999. V52. P305 HCAPLUS

(5) Hawser, S; J Clin Microbiol 1998. V36. P1450 HCAPLUS

(6) Hawser, S; J Med Vet Mycol 1996. V34. P149 MEDLINE

(7) Jahn, B; J Clin Microbiol 1996. V34. P2039 HCAPLUS

(8) Kurtz, M; Antimicrob Agents Chemother 1994. V38. P1480 HCAPLUS

(9) Kurtz, M; J Med Vet Mycol 1997. V35. P79 MEDLINE

(10) Latge, J; Clin Microbiol Rev 1999. V12. P310 MEDLINE

(11) Mukhopadhyay, T; J Antibiot (Tokyo) 1987. V40. P281 HCAPLUS

(12) National Committee for Clinical Laboratory Standards; Reference method for broth dilution antifungal susceptibility testing of conidium-forming filamentous fungi. Proposed standard M38-P 1998

(13) Roy, K; J Antibiot (Tokyo) 1987. V40. P275 HCAPLUS

(14) Tellier, R; Antimicrob Agents Chemother 1992. V36. P1619 HCAPLUS

(15) Tiballi, R; J Clin Microbiol 1995. V33. P915 HCAPLUS

IT 108351-20-8. Mulundocandin

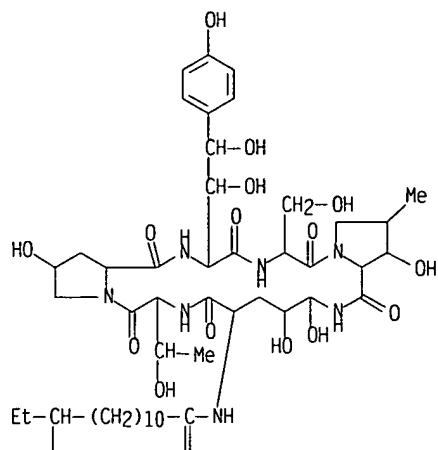
RL: BSU (Biological study, unclassified); BIOL (Biological study)

(utility of XTT and min. effective concentration assays in the determination of antifungal susceptibility of *Aspergillus fumigatus* to the lipopeptide class of compds.)

RN 108351-20-8 HCAPLUS

CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L17 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:708788 HCAPLUS
 DN 131:322923
 ED Entered STN: 05 Nov 1999
 TI A process for the conversion of echinocandin class of peptides to their
 C4-homotyrosine monodeoxy analogs
 IN Mukhopadhyay, Triptikumar; Jayvanti, Kenia; Kumar, Erra Koteswara Satya
 Vijaya
 PA Hoechst Marion Roussel Deutschland GmbH, Germany
 SO PCT Int. Appl.. 18 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07K007-56
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9955727	A1	19991104	WO 1999-EP2715	19990422
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2327474	AA	19991104	CA 1999-2327474	19990422
AU 9937096	A1	19991116	AU 1999-37096	19990422
AU 758395	B2	20030320		
BR 9909853	A	20001219	BR 1999-9853	19990422
TR 200003058	T2	20010122	TR 2000-200003058	19990422
EP 1073675	A1	20010207	EP 1999-919261	19990422

102 (c)

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,
SI, LT, LV, FI, RO

EE 200000611	A	20020415	EE 2000-611	19990422
JP 2002513033	T2	20020508	JP 2000-545885	19990422
AP 1111	A	20021023	AP 2000-200001894	19990422

W: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW

NZ 506667	A	20030228	NZ 1999-506667	19990422
CZ 293547	B6	20040616	CZ 2000-3903	19990422
ZA 2000004600	A	20011127	ZA 2000-4600	20000901
BG 104772	A	20010430	BG 2000-104772	20000918
NO 2000005258	A	20001019	NO 2000-5258	20001019
HR 2000000719	A1	20011031	HR 2000-719	20001023
US 6809177	B1	20041026	US 2001-673836	20010329

PRAI EP 1998-107397 A 19980423
WO 1999-EP2715 W 19990422

No 100 (a)

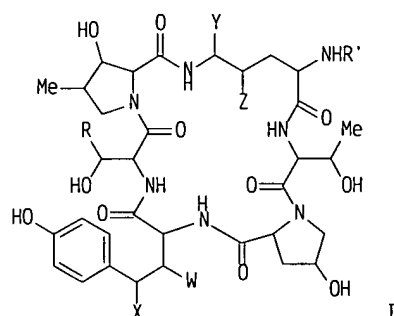
CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 9955727	ICM	C07K007-56
WO 9955727	ECLA	C07K007/56
US 6809177	ECLA	C07K007/56

OS CASREACT 131:322923; MARPAT 131:322923

GI



AB Echinocandin type peptides I (X = OH; W, Y, Z = OH; H; R = Me, CH₂CONH₂, H; R' = linoleoyl, 10.12-dimethylmyristoyl, 12-methyltetradecanoyl) were converted to their C4-homotyrosine (C4-htyr) monodeoxy analogs I (X = H) via a single step selective reduction of the C4-htyr hydroxyl group of echinocandins to their monodeoxy analogs under neutral conditions without prior protection/deprotection of the equally facile C5-Orn (ornithine) hydroxyl group and purification of the monodeoxy compound from the crude reaction mixture. Thus, a mixture of mulundocandin and Raney nickel in a pH 7 ethanol solution was stirred for 3 h at room temperature to afford 30% deoxymulundocandin, following purification by liquid-liquid chromatog.

ST peptide echinocandin redn: deoxyechinocandin prepn

IT Peptides, preparation

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for conversion of echinocandin class of peptides to their C4-homotyrosine monodeoxy analogs)

IT 54651-05-7, Echinocandin b 108351-20-8, Mulundocandin

120692-19-5, Pneumocandin a0 135575-42-7, Pneumocandin b0 135862-90-7,

Pneumocandin A1 135867-75-3, Pneumocandin a2 138530-80-0, Pneumocandin

B2 144074-96-4, Pneumocandin c0

RL: RCT (Reactant); RACT (Reactant or reagent)

(process for conversion of echinocandin class of peptides to their C4-homotyrosine monodeoxy analogs)

IT 71018-12-7P, Echinocandin c 138626-63-8P, Deoxymulundocandin

144448-05-5P. Deoxypneumocandin B0 144476-69-7P. Deoxypneumocandin A2
 248281-21-2P. Deoxypneumocandin A0 248281-23-4P. Deoxypneumocandin A1
 248281-27-8P. Deoxypneumocandin B2 248281-29-0P. Deoxypneumocandin C0

RL: SPN (Synthetic preparation); PREP (Preparation)

(process for conversion of echinocandin class of peptides to their
 C4-homotyrosine monodeoxy analogs)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Balkovec. J: WO 9608266 A 1996 HCAPLUS
- (2) Balkovec. J: Tetrahedron Letters 1992. V33(32). P4529
- (3) Fujisawa Pharmaceutical Co: EP 0644199 A 1995 HCAPLUS
- (4) Merck & Co Inc: EP 0459564 A 1991 HCAPLUS
- (5) Merck & Co Inc: EP 0535959 A 1993 HCAPLUS
- (6) Merck & Co Inc: EP 0535968 A 1993 HCAPLUS

IT 108351-20-8. Mulundocandin

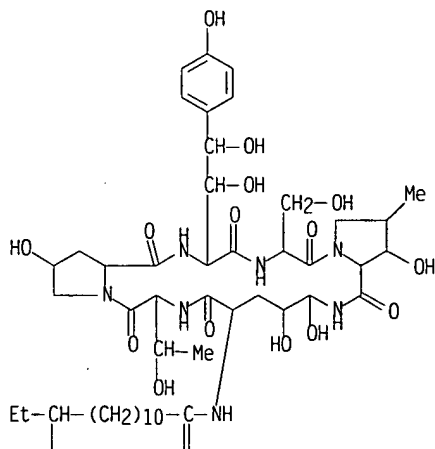
RL: RCT (Reactant); RACT (Reactant or reagent)

(process for conversion of echinocandin class of peptides to their
 C4-homotyrosine monodeoxy analogs)

RN 108351-20-8 HCAPLUS

CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L17 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:215237 HCAPLUS

DN 131:2688

ED Entered STN: 06 Apr 1999

TI Comparisons of the effects of fungicidal and fungistatic antifungal agents
 on the morphogenetic transformation of Candida albicans

AU Hawser, Stephen; Islam, Khalid

CS Hoechst Marion Roussel, Romainville. 93235. Fr.

SO Journal of Antimicrobial Chemotherapy (1999). 43(3). 411-413

CODEN: JACHDX; ISSN: 0305-7453

PB Oxford University Press

DT Journal

LA English

For.

CC 10-5 (Microbial, Algal, and Fungal Biochemistry)

AB Eleven different antifungal agents were compared, and their ability to inhibit the morphogenetic transformation of *Candida albicans* was examined together with their ability to inhibit growth, as measured by MIC methodol. The fungicidal potential of each agent was also determined. Of the antifungal agents tested, only amphotericin B, mulundocandin and aculeacin inhibited the transformation at sub-MIC values; all three agents showed fungicidal activity at concns. close to the MIC. All other agents were fungicidal only at concns. much higher than the MIC and inhibited the morphogenetic transformation only at concns. above the MIC. These data suggest that fungicidal antifungal agents are more likely to act by inhibiting the morphogenetic transformation of *C. albicans* while fungistatic agents are unable to do so and are more likely to block growth by budding.

ST *Candida* morphogenetic transformation antifungal agent

IT *Candida albicans*
Fungicides
(comparisons of effects of fungicidal and fungistatic antifungal agents on morphogenetic transformation of *Candida albicans*)

IT Development, microbial
(dimorphism; comparisons of effects of fungicidal and fungistatic antifungal agents on morphogenetic transformation of *Candida albicans*)

IT 1397-89-3, Amphotericin B 2022-85-7, Flucytosine 11089-65-9, Tunicamycin 22916-47-8, Miconazole 60606-49-7, Aculeacin 65277-42-1 78613-35-1, Amorolfine 84625-61-6, Itraconazole 86386-73-4, Fluconazole 91161-71-6, Terbinafine 108351-20-8, Mulundocandin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(comparisons of effects of fungicidal and fungistatic antifungal agents on morphogenetic transformation of *Candida albicans*)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Hawser, S: Journal of Antimicrobial Chemotherapy 1996, V38, P579 HCAPLUS

(2) Kerridge, D: Advances in Microbial Physiology 1986, V27, P1 HCAPLUS

(3) Kurtz, M: Antimicrobial Agents and Chemotherapy 1994, V38, P1480 HCAPLUS

(4) Lo, H: Cell 1997, V90, P939 HCAPLUS

(5) National Committee For Clinical Laboratory Standards: Reference Method for Broth Dilution Antifungal Susceptibility Testing of Yeasts: Tentative Standard M27-T 1995

(6) Odds, F: *Candida* and Candidosis 2nd edn 1988

(7) Ryder, N: Annals of the New York Academy of Sciences 1988, V544, P208 HCAPLUS

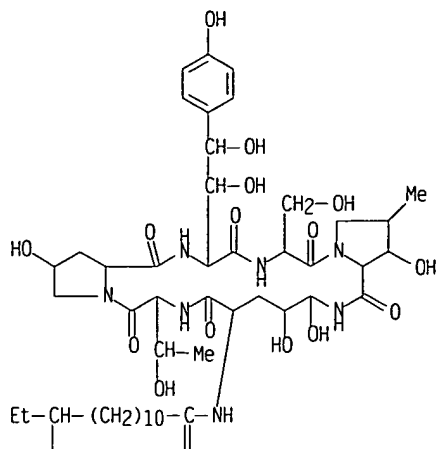
(8) Vanden, B: Sterol Biosynthesis Inhibitors: Pharmaceutical and Agrochemical Aspects 1988, P79

IT 108351-20-8, Mulundocandin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(comparisons of effects of fungicidal and fungistatic antifungal agents on morphogenetic transformation of *Candida albicans*)

RN 108351-20-8 HCAPLUS

CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L17 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:214634 HCAPLUS
 DN 131:2683
 ED Entered STN: 06 Apr 1999
 TI Mulundocandin, an echinocandin-like lipopeptide antifungal agent:
 biological activities in vitro
 AU Hawser, Stephen; Borgonovi, Monica; Markus, Astrid; Isert, Dieter
 CS Hoechst Marion Roussel, Romainville, F-93235, Fr.
 SO Journal of Antibiotics (1999), 52(3), 305-310
 CODEN: JANTAJ; ISSN: 0021-8820
 PB Japan Antibiotics Research Association
 DT Journal
 LA English
 CC 10-5 (Microbial, Algal, and Fungal Biochemistry)
 AB Mulundocandin (MCN) is an antifungal lipopeptide which belongs to the
 echinocandin class of antimycotic agents. MCN exhibited good in vitro
 activity against *Candida albicans* and *C. glabrata* isolates with MIC ranges
 of 0.5.apprx.4.0 µg/mL and 2.0.apprx.4.0 µg/mL, resp. MCN also
 exhibited some activity against *C. tropicalis* isolates (MIC range
 1.0.apprx.8.0 µg/mL). However, MCN was poorly active against other
 non-albicans isolates and was inactive against *Cryptococcus neoformans*,
Aspergillus species and *Trichophyton*. MCN appeared to exert its
 antifungal activity through preferential inhibition of germ tube formation
 (MIC-HY 0.015.apprx.0.03 µg/mL) and was typically less active on the
 yeast form (MIC 0.5.apprx.4.0 µg/mL). In kill-curve expts. 99.9%
 redns. in cell viability were observed following 8 h exposure to MCN at 4
 + MIC and 8 + MIC and after 5 h exposure to 16 + MIC.
 ST mulundocandin antifungal action *Candida*
 IT Fungicides
 (action mechanism; biol. activities of the echinocandin-like
 lipopeptide antifungal agent mulundocandin in vitro)
 IT *Candida albicans*
Candida glabrata
Candida tropicalis

for.

(biol. activities of the echinocandin-like lipopeptide antifungal agent mulundocandin in vitro)

IT Morphogenesis, microbial

(germ tube formation; biol. activities of the echinocandin-like lipopeptide antifungal agent mulundocandin in vitro)

IT Blood serum

(mulundocandin antifungal activity sensitivity to)

IT 108351-20-8. Mulundocandin

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use);

BIOL (Biological study); PROC (Process); USES (Uses)

(biol. activities of the echinocandin-like lipopeptide antifungal agent mulundocandin in vitro)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Balkovec, J: Exp Opin Invest Drugs 1994, V3, P65 HCAPLUS

(2) Fan Harvard, P: Antimicrob Agents Chemother 1991, V35, P2302

(3) Frosco, M: Exp Opin Invest Drugs 1997, V6, P1951 HCAPLUS

(4) Hawser, S: J Antimicrob Chemother 1996, V38, P67 HCAPLUS

(5) Klepser, M: Diagn Microbiol Infect Dis 1997, V29, P227 HCAPLUS

(6) Mukhopadhyay, T: J Antibiotics 1992, V45, P618 HCAPLUS

(7) National Committee for Clinical Laboratory Standards: Reference method for broth dilution antifungal susceptibility testing of yeast: approved standard 1997

(8) Ruhnke, M: J Clin Microbiol 1994, V32, P2092 MEDLINE

(9) Schmatz, D: J Antibiotics 1992, V45, P1886 HCAPLUS

(10) Takesako, K: J Antibiotics 1991, V44, P919 HCAPLUS

IT 108351-20-8. Mulundocandin

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use);

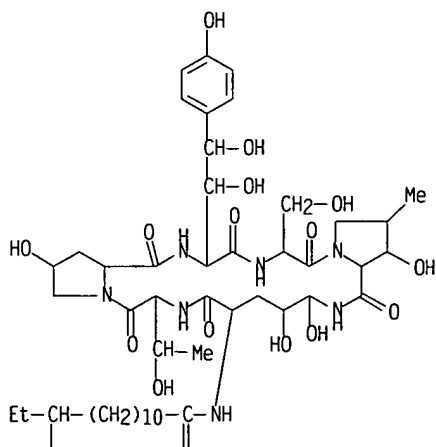
BIOL (Biological study); PROC (Process); USES (Uses)

(biol. activities of the echinocandin-like lipopeptide antifungal agent mulundocandin in vitro)

RN 108351-20-8 HCAPLUS

CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



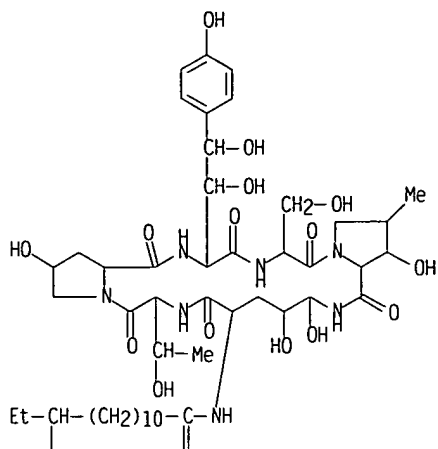
PAGE 2-A



L17 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1990:95331 HCAPLUS
 DN 112:95331
 ED Entered STN: 18 Mar 1990
 TI Synthesis and evaluation of LY121019, a member of a series of
 semisynthetic analogs of the antifungal lipopeptide echinocandin B
 AU Debono, M.; Abbott, B. J.; Turner, J. R.; Howard, L. C.; Gordee, R. S.;
 Hunt, A. S.; Barnhart, M.; Molloy, R. M.; Willard, K. E.; et al.
 CS Lilly Res. Lab., Lilly Corporate Cent., Indianapolis, IN. 46285, USA
 SO Annals of the New York Academy of Sciences (1988), 544(Antifungal Drugs),
 152-67
 CODEN: ANYAA9; ISSN: 0077-8923
 DT Journal
 LA English
 CC 10-5 (Microbial Biochemistry)
 AB The lipopeptide antibiotic echinocandin B (ECB) was efficiently deacylated
 by *Actinoplanes utahensis*. The resulting deacylated peptide was
 reacylated to give an extensive series of semisynthetic ECB analogs having
 interesting anti-*Candida* activity. The improved biol. properties of these
 analogs led to the selection of LY121019 for further evaluation as a
 potential therapeutic agent for disseminated candidiasis.
 ST antibiotic LY12109 fungicide echinocandin B analog: *Candida* LY12109
 echinocandin B analog
 IT *Actinoplanes utahensis*
 (echinocandin B deacylation by)
 IT Fungicides and Fungistats
 (medical, echinocandin B analogs as)
 IT 54651-05-7, Echinocandin B 54651-05-7D, Echinocandin B, analogs
 54651-06-8 58814-86-1 79404-92-5 79565-23-4 79565-25-6
 79565-36-9 79565-37-0 79565-38-1 79565-39-2 79784-90-0
 79784-91-1 79784-93-3 79784-98-8 79784-99-9 79785-01-6
 79785-11-8 79785-12-9 79785-13-0 79785-14-1 79785-15-2
 79785-16-3 79785-17-4 79785-18-5 79785-19-6 79785-20-9
 79785-22-1 79785-23-2 79785-24-3 79785-25-4 79785-27-6
 79785-29-8 79785-30-1 79785-32-3 79785-33-4 79785-34-5
 79785-35-6 79785-38-9 79785-40-3 79785-42-5 79785-44-7
 79794-87-9 79932-13-1 79951-37-4 82029-17-2, Antibiotic S 41062F1
 108351-20-8 121150-24-1 121150-25-2 124278-01-9
 125211-04-3 125211-05-4
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); BIOL (Biological study)
 (antifungal activity of)
 IT 79404-91-4, LY121019
 RL: BIOL (Biological study)
 (synthesis and antifungal activity of)
 IT 108351-20-8
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); BIOL (Biological study)
 (antifungal activity of)
 RN 108351-20-8 HCAPLUS
 CN Mulundocandin (9CI) (CA INDEX NAME)

102 (b)

PAGE 1-A



PAGE 2-A



L17 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1989:552145 HCAPLUS
 DN 111:152145
 ED Entered STN: 28 Oct 1989
 TI Manufacture of novel antibiotic mulundocandin with *Aspergillus sydowii*
 IN Roy, Kirity; Reddy, Goukanapalli Chandrasekh; Mukhopadhyay, Triptikumar;
 Ganguli, Bimal Naresh; Desikan, Kalyania Puram Rajagop
 PA Hoechst India Ltd., India
 SO Indian 40 pp.
 CODEN: INXXAP
 DT Patent
 LA English
 IC ICM C12D009-22
 CC 16-2 (Fermentation and Bioindustrial Chemistry)
 FAN.CNT 1

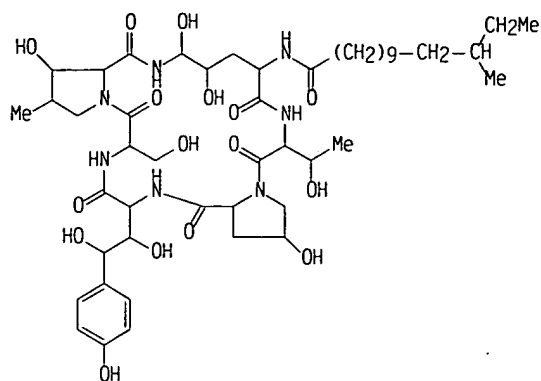
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI IN 162032	A	19880319	IN 1985-B022	19850121
PRAI IN 1985-B022		19850121		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
IN 162032	ICM	C12D009-22

GI

Indian Pat
Couldnt call up.



AB Antibiotic mulundocandin (I) is manufactured by fermentation of a novel *Aspergillus sydowii* strain. The *A. sydowii* strain was cultured for 76 h at 26° in medium containing beef extract, tryptones, glucose, soluble starch, yeast extract, and salts, pH 6.5. I was purified from a MeOH extract of the mycelia and an EtOAc extract of the culture filtrate by silica gel and Sephadex LH-20 column chromatog., and silica gel TLC. The physicochem. characteristics of I were determined (m.p.; solubility; sp. rotation; and mass, UV, IR, and NMR spectra). I displayed anti-yeast and antifungal activities.

ST mulundocandin fungicide fermn *Aspergillus*

IT Molecular structure, natural product
(mulundocandin (fatty acyl peptide))

IT *Aspergillus sydowii*

(mulundocandin fungicide manufacture with)

IT Fermentation

(mulundocandin fungicide, with *Aspergillus sydowii*)

IT Fungicides and Fungistats

(mulundocandin, from *Aspergillus sydowii*)

IT 108351-20-8P, Mulundocandin

RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)

(manufacture of, with *Aspergillus sydowii*)

IT 108351-20-8P, Mulundocandin

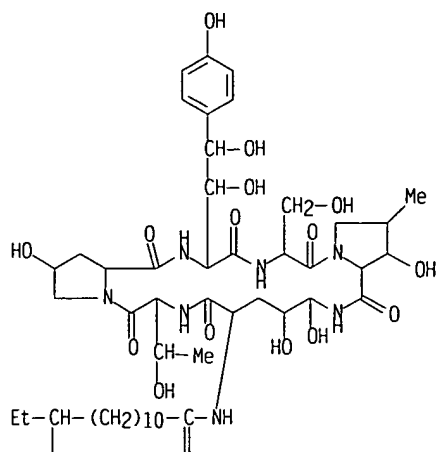
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)

(manufacture of, with *Aspergillus sydowii*)

RN 108351-20-8 HCAPLUS

CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A

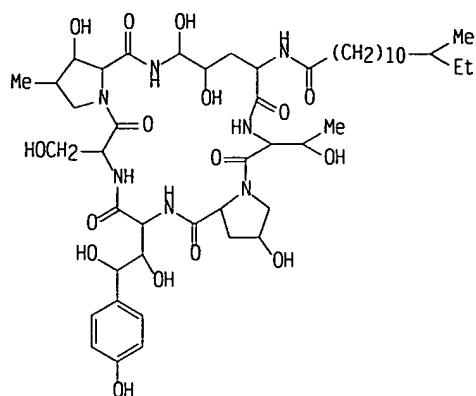


PAGE 2-A



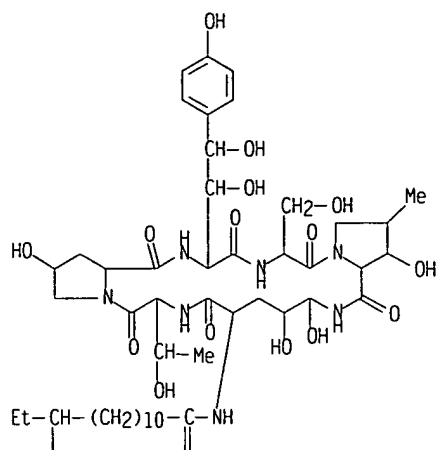
L17 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1988:38346 HCAPLUS
 DN 108:38346
 ED Entered STN: 06 Feb 1988
 TI Mulundocandin, a new lipopeptide antibiotic. II. Structure elucidation
 AU Mukhopadhyay, Triptikumar; Ganguli, B. N.; Fehlhaber, H. W.; Kogler, H.;
 Vertesy, L.
 CS Res. Cent., Hoechst India Ltd., Bombay, 400 080, India
 SO Journal of Antibiotics (1987), 40(3), 281-9
 CODEN: JANTAJ; ISSN: 0021-8820
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 22
 OS CASREACT 108:38346
 GI

(02/b)



- AB Mulundocandin, a new antifungal antibiotic, was shown to have structure I by high field NMR expts., e.g., homo- and heteronuclear correlation spectra, distortionless enhancement by polarization transfer (DEPT) spectra as well as nuclear Overhauser effect. The compound is a lipopeptide belonging to the echinocandin class.
- ST mulundocandin lipopeptide structure NMR
- IT Molecular structure, natural product
(of mulundocandin (lipopeptide antibiotic))
- IT Molecular structure-property relationship
(NMR, mulundocandin)
- IT 5502-94-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in hydrolysis of mulundocandin)
- IT 108351-20-8, Mulundocandin
RL: PROC (Process)
(mol. structure determination of)
- IT 5129-66-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mass spectrum of)
- IT 112159-10-1P 112159-11-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 108351-20-8, Mulundocandin
RL: PROC (Process)
(mol. structure determination of)
- RN 108351-20-8 HCAPLUS
- CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A

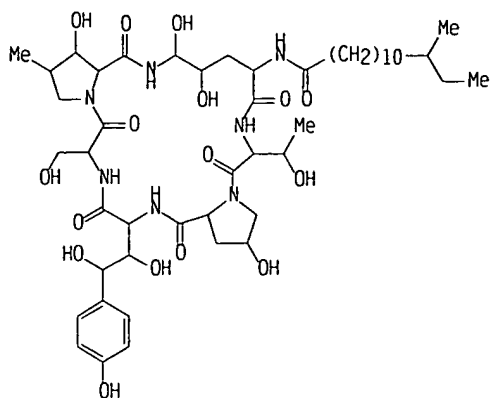


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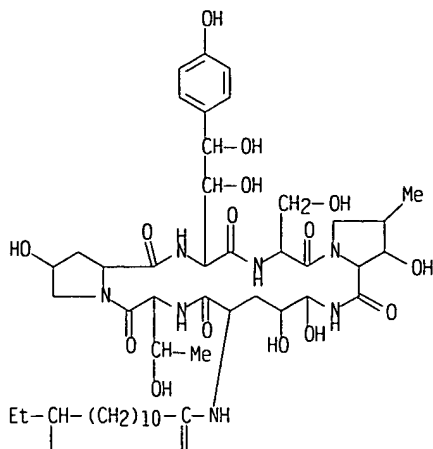
L17 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1987:210646 HCAPLUS
 DN 106:210646
 ED Entered STN: 26 Jun 1987
 TI Mulundocandin, a new lipopeptide antibiotic. I. Taxonomy, fermentation, isolation, and characterization
 AU Roy, Kirity; Mukhopadhyay, Triptikumar; Reddy, G. C. S.; Desikan, K. R.; Ganguli, B. N.
 CS Res. Cent., Hoechst India Ltd., Bombay, 400 080, India
 SO Journal of Antibiotics (1987), 40(3), 275-80
 CODEN: JANTAJ; ISSN: 0021-8820
 DT Journal
 LA English
 CC 10-1 (Microbial Biochemistry)
 Section cross-reference(s): 26
 GI

102(b)



- AB Mulundocandin (I), a new lipopeptide antibiotic, was isolated from the culture broth of a strain of *Aspergillus sydowi* Number Y-30462. The antibiotic, obtained as a colorless amorphous powder having the mol. formula $C_{48}H_{77}N_7O_{16}$, is an antifungal antibiotic active against yeasts and filamentous fungi.
- ST *Aspergillus* antibiotic lipopeptide fungicide
- IT *Aspergillus sydowi*
(antibiotic from, mulundocandin as)
- IT Lipopeptides
RL: BIOL (Biological study)
(antibiotic, from *Aspergillus sydowi*, isolation and structure of)
- IT Antibiotics
Fungicides and Fungistats
(from *Aspergillus sydowi*, mulundocandin as)
- IT Nomenclature, new natural products
(mulundocandin (lipopeptide))
- IT Molecular structure, natural product
(of mulundocandin (lipopeptide))
- IT 108351-20-8
RL: BIOL (Biological study)
(antibiotic, from *Aspergillus sydowi*, isolation and structure of)
- IT 108351-20-8
RL: BIOL (Biological study)
(antibiotic, from *Aspergillus sydowi*, isolation and structure of)
- RN 108351-20-8 HCAPLUS
- CN Mulundocandin (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



=> d all hitstr 128 tot

L28 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:488724 HCAPLUS

DN 133:267119

ED Entered STN: 19 Jul 2000

TI Total synthesis and antifungal evaluation of cyclic aminohexapeptides

AU Klein, Larry L.; Li, Leping; Chen, Hui-Ju; Curty, Cynthia B.; DeGoey,
David A.; Grampovnik, David J.; Leone, Christina L.; Thomas, Sheela A.;
Yeung, Clinto M.; Funk, Kenneth W.; Kishore, Vimal; Lundell, Edwin O.;
Wodka, Dariusz; Meulbroek, Jon A.; Alder, Jeffrey D.; Nilius, Angela M.;
Lartey, Paul A.; Plattner, Jacob J.

CS Infectious Disease Research, Abbott Laboratories, Abbott Park, IL,
60064-3500, USA

SO Bioorganic & Medicinal Chemistry (2000), 8(7), 1677-1696
CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

LA English

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1

OS CASREACT 133:267119

AB Naturally occurring hexapeptide echinocandin B (1) has shown potent
antifungal activity via its inhibition of the synthesis of β -1,3
glucan, a key fungal cell wall component. Although this series of agents
has been limited thus far based on their physicochem. characteristics, we
have found that the synthesis of analogs bearing an aminoproline residue
in the 'northwest' position imparts greatly improved water solubility (>5
mg/mL). The synthesis and structure-activity relationships (SAR) based on
whole cell and upon in vivo activity of the series of compds. are
reported.

ST cyclic aminohexapeptide prepn MSBAR fungicide Candida

IT Candida

Search done by Noble Jarrell

(antifungal evaluation of cyclic aminohexapeptides against *C. albicans* and *C. glabrata*)

IT Peptides, preparation

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(cyclic: total synthesis and antifungal evaluation of cyclic aminohexapeptides)

IT Cyclization

Fungicides

Structure-activity relationship

(total synthesis and antifungal evaluation of cyclic aminohexapeptides)

IT	200265-27-6P	200265-28-7P	200265-29-8P	200265-30-1P	200265-32-3P
	200265-33-4P	200265-35-6P	200265-36-7P	200265-37-8P	200265-42-5P
	200265-43-6P	200265-50-5P	200265-55-0P	200265-63-0P	200265-69-6P
	200265-85-6P	200265-88-9P	200265-93-6P	200265-96-9P	200266-02-0P
	296774-28-2P	296774-31-7P	296774-34-0P	296774-36-2P	296774-38-4P
	296774-40-8P	296774-42-0P	296774-43-1P	296774-45-3P	
	296774-73-7P	296774-75-9P	296774-77-1P	296774-79-3P	
	296774-81-7P	296774-85-1P	296774-89-5P	296774-93-1P	296775-16-1P
	296775-18-3P	296775-21-8P	296775-40-1P	296775-41-2P	296775-42-3P
	296775-43-4P	296775-44-5P	296775-48-9P	296775-49-0P	296775-50-3P
	296775-51-4P	296775-52-5P	296775-53-6P	296775-54-7P	296775-55-8P
	296775-56-9P	296775-57-0P			

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(total synthesis and antifungal evaluation of cyclic aminohexapeptides)

IT	50-00-0, Formaldehyde, reactions	95-95-4, 2,4,5-Trichlorophenol
	100-52-7, Benzaldehyde, reactions	115-11-7, Isobutylene, reactions
	124-07-2, Octanoic acid, reactions	124-13-0, Octanal
	2592-18-9	2812-46-6 3256-45-9 3262-72-4 3304-51-6 3978-80-1
	4326-36-7	4530-20-5 13726-76-6 13734-40-2 19728-63-3 21887-64-9
	23680-31-1	30992-29-1 34306-42-8 47173-80-8 55674-67-4
	62147-27-7	71989-31-6 71989-35-0 73259-81-1 74844-91-0
	86069-86-5	88050-17-3 93527-54-9 100564-78-1 122996-47-8
	141899-12-9	150828-96-9 158937-65-6 198473-94-8 221243-01-2
	296774-32-8	296774-39-5 296774-64-6 296775-06-9 296775-17-2
	296775-19-4	296775-22-9 296775-23-0 296775-24-1 296775-25-2
	296775-26-3	296775-27-4 296775-28-5 296775-29-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(total synthesis and antifungal evaluation of cyclic aminohexapeptides)

IT	84520-67-2P	84520-68-3P	112766-18-4P	118433-97-9P	123993-33-9P
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	198560-10-0P	221243-01-2DP, resin-bound	263846-84-0P	263846-85-1P	
	263846-87-3P	263846-88-4P	263846-89-5P	263846-91-9P	263846-92-0P
	263846-94-2P	263847-08-1P	296774-19-1P	296774-20-4P	296774-21-5P
	296774-22-6P	296774-23-7P	296774-24-8P	296774-25-9P	296774-26-0P
	296774-27-1P	296774-29-3DP, resin-bound	296774-30-6P	296774-33-9P	
	296774-35-1P	296774-37-3P	296774-41-9P	296774-44-2P	296774-46-4P
	296774-47-5P	296774-49-7DP, resin-bound	296774-50-0DP, resin-bound		
	296774-51-1P	296774-52-2P	296774-53-3P	296774-54-4P	296774-55-5P
	296774-56-6P	296774-57-7P	296774-58-8P	296774-59-9P	296774-60-2P
	296774-61-3P	296774-62-4P	296774-63-5P	296774-65-7P	296774-66-8P
	296774-67-9P	296774-68-0P	296774-69-1P	296774-70-4P	296774-71-5P
	296774-72-6P	296774-74-8P	296774-76-0P	296774-78-2P	
	296774-80-6P	296774-82-8P	296774-87-3P	296774-91-9P	296774-95-3P
	296774-96-4P	296774-98-6P	296775-00-3P	296775-04-7P	296775-08-1P
	296775-11-6P	296775-13-8P	296775-15-0P	296775-20-7P	296775-30-9P
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	296775-59-2P	296775-60-5P	296775-61-6P	296775-62-7P	296775-63-8P
	296775-64-9P	296775-65-0P	296775-66-1P	296775-67-2P	296775-68-3P
	296775-69-4P				

RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)

(total synthesis and antifungal evaluation of cyclic aminohexapeptides)

IT 216774-50-4P 296774-48-6P

RL: SPN (Synthetic preparation): PREP (Preparation)

(total synthesis and antifungal evaluation of cyclic aminohexapeptides)

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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IT 296774-73-7P

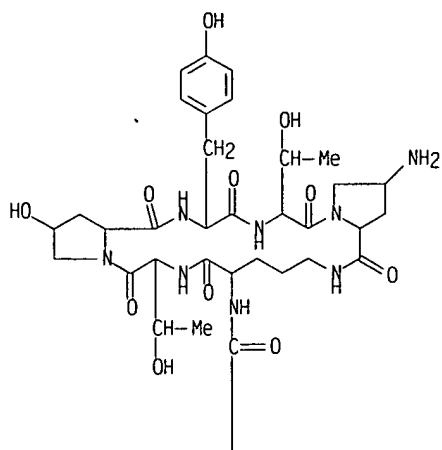
RL: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation)

(total synthesis and antifungal evaluation of cyclic aminohexapeptides)

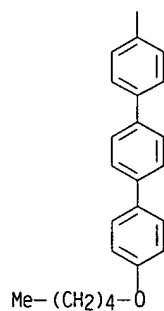
RN 296774-73-7 HCAPLUS

CN Echinocandin B, 1-[N2-[[4''-(pentyloxy)[1,1':4'.1''-terphenyl]-4-yl]carbonyl]-L-ornithine]-4-L-tyrosine-6-[(4S)-4-amino-L-proline]- (9CI)
(CA INDEX NAME)

PAGE 1-A

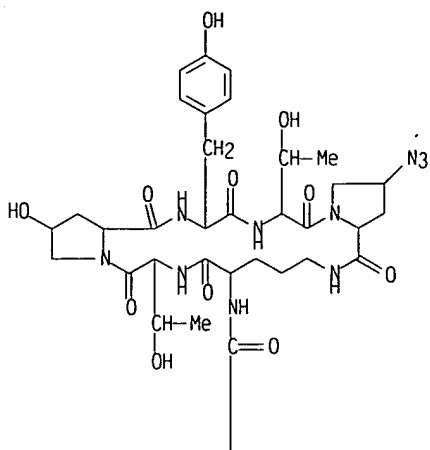


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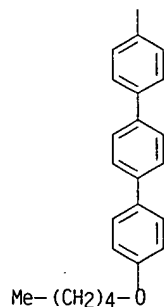


IT 296774-74-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (total synthesis and antifungal evaluation of cyclic aminohexapeptides)
 RN 296774-74-8 HCAPLUS
 CN Echinocandin B. 1-[N²-[[4''-(pentyloxy)[1,1':4'.1''-terphenyl]-4-
 yl]carbonyl]-L-ornithine]-4-L-tyrosine-6-[(4S)-4-azido-L-proline]- (9CI)
 (CA INDEX NAME)

PAGE 1-A

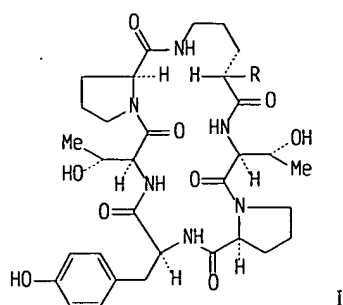


PAGE 2-A



L28 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1992:470296 HCAPLUS
 DN 117:70296
 ED Entered STN: 23 Aug 1992
 TI Preparation and structure-activity relationships of simplified analogs of
 the antifungal agent cilofungin: a total synthesis approach
 AU Zambias, Robert A.; Hammond, Milton L.; Heck, James V.; Bartizal, Ken;
 Trainor, Charlotte; Abruzzo, George; Schmatz, Dennis M.; Nollstadt, Karl
 M.
 CS Merck Res. Lab., Rahway, NJ, 07065, USA
 SO Journal of Medicinal Chemistry (1992), 35(15), 2843-55
 CODEN: JMCMAR; ISSN: 0022-2623
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 10
 OS CASREACT 117:70296
 GI

102 (b)



AB The echinocandins are a well-known class of lipopeptides characterized by their potent antifungal activity against *Candida* species. The mechanism of action of the echinocandins is generally thought to be the inhibition of β -1,3-glucan synthesis, an important structural component in the cell wall of *Candida* species. Extensive structure-activity studies on the fatty acid side chain of echinocandin B led to the preparation of the clin. candidate cilofungin. We now report the preparation, by solid-phase synthesis, of a series of simplified analogs of cilofungin in which the unusual amino acids found in the echinocandins were replaced with more readily accessible natural amino acids. The solid-phase approach to the total synthesis of these analogs allowed us to conveniently explore structural modifications that could not be accomplished by chemical modification of the natural product. The simplest analog I [R = p-[Me(CH₂)₇O]C₆H₄CONH] showed no biol. activity. Structural complexity was then returned to the system in a systematic fashion so as to reapproach the original cilofungin structure. Antifungal activity and the inhibition of β -1,3-glucan synthesis were monitored at each step of the process, thereby revealing the basic structure-activity relationships of the amino acids and the minimal structural requirements for biol. activity in the echinocandin ring system. The results suggests that the 3-hydroxy-4-methylproline residue enhances activity but the L-homotyrosine residue is crucial for both antifungal activity and the inhibition of β -1,3-glucan synthesis.

ST cilofungin analog prepn antifungal; structure activity relationship
antifungal cilofungin analog

IT Fungicides and Fungistats

(cilofungin simplified analogs)

IT Molecular structure-biological activity relationship
(fungicidal, of cilofungin simplified analogs)

IT 501-53-1. Benzyloxycarbonyl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(benzyloxycarbonylation by, ornithine-containing peptides)

IT 110936-12-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(deblocking of)

IT 109425-55-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(esterification of, with pentachlorophenol)

IT 2493-84-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(esterification of, with pentafluorophenol)

IT 111002-66-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of, with pentapeptide derivative)

IT 106159-24-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acylation by, of ornithine-containing peptides)

IT 79404-91-4DP, Cilofungin, simplified analogs 141806-00-0P

141806-09-9P 141806-10-2P 141806-11-3P
 141806-12-4P 141806-13-5P 141806-14-6P 141806-15-7P 141806-25-9P
 141806-32-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and antifungal activity of)

IT 141806-18-0P 141806-26-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and benzyloxycarbonylation of)

IT 141806-01-1P 141806-02-2P 141806-03-3P 141806-04-4P 141806-05-5P
 141806-06-6P 141806-07-7P 141806-08-8P 141806-24-8P 141806-31-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of)

IT 141806-23-7P 141806-30-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrogenolysis of)

IT 141806-19-1P 141806-20-4P 141806-27-1P 141806-28-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and peptide coupling of, with proline derivative)

IT 141806-21-5P 141806-22-6P 141806-29-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and saponification of)

IT 123180-69-8P 141806-17-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and solid-phase peptide coupling of)

IT 54631-81-1DP, resin-bound
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and solid-phase peptides synthesis with)

IT 141899-12-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and O-benylation of, with trichlorobenzyl bromide)

IT 141806-16-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and tert-butoxycarbonylation of)

IT 15260-10-3 15761-39-4, N-tert-Butoxycarbonyl-L-proline 47689-67-8
 54631-81-1 86060-90-4 86060-93-7 118554-00-0 119767-84-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (solid-phase peptide coupling of)

IT 15260-10-3D, resin-bound 15761-39-4D, N-tert-Butoxycarbonyl-L-proline, resin-bound 71989-31-6D, resin-bound
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (solid-phase peptide synthesis with)

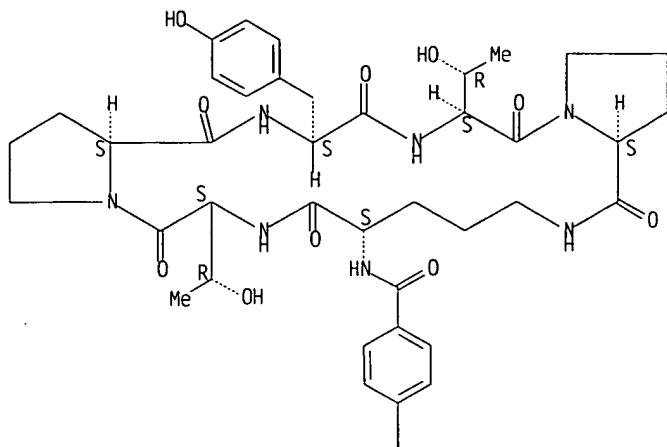
IT 20443-98-5, 2,6-Dichlorobenzyl bromide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (O-benylation by, of homotyrosine derivative)

IT 141806-00-0P 141806-09-9P 141806-10-2P
 141806-11-3P 141806-32-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and antifungal activity of)

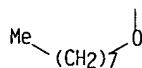
RN 141806-00-0 HCAPLUS
 CN L-Proline, N2-[4-(octyloxy)benzoyl]-L-ornithyl-L-threonyl-L-prolyl-L-tyrosyl-L-threonyl-, cyclic (6+1)-peptide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



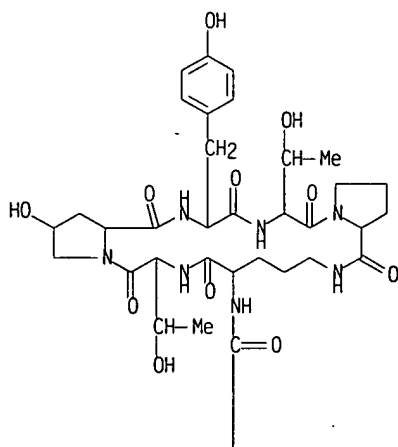
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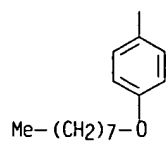
RN 141806-09-9 HCAPLUS

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PAGE 1-A



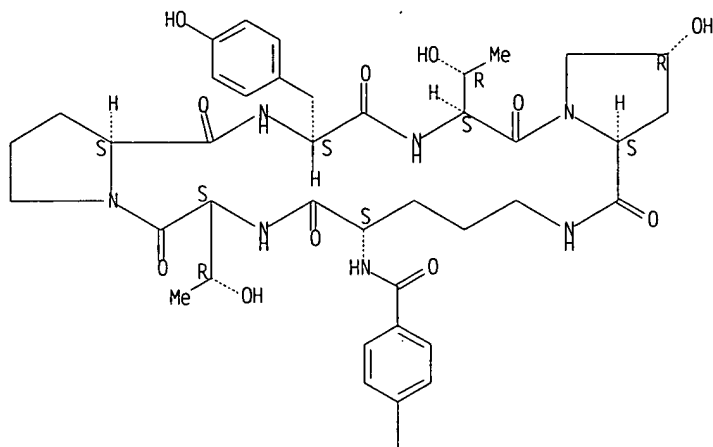
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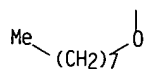
RN 141806-10-2 HCAPLUS
 CN L-Proline, N2-[4-(octyloxy)benzoyl]-L-ornithyl-L-threonyl-L-prolyl-L-tyrosyl-L-threonyl-4-hydroxy-, cyclic (6+1)-peptide, trans- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

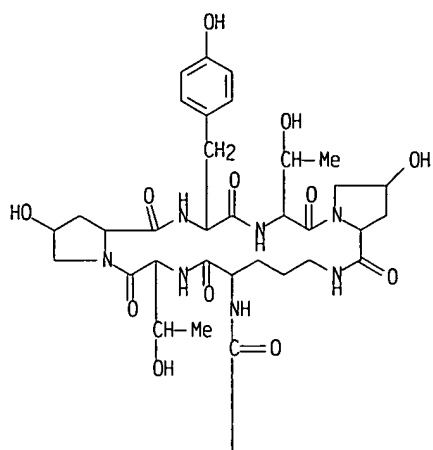


PAGE 2-A

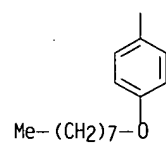


RN 141806-11-3 HCAPLUS
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PAGE 1-A

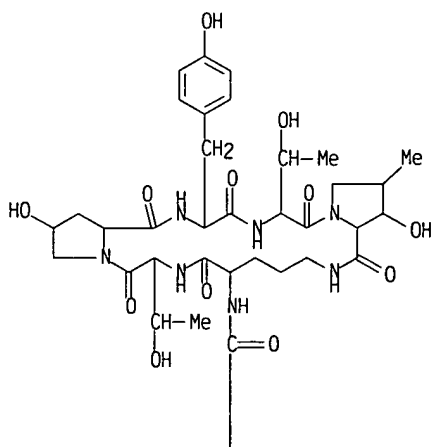


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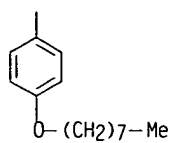


RN 141806-32-8 HCAPLUS
CN Echinocandin B. 1-[N2-[4-(octyloxy)benzoyl]-L-ornithine]-4-L-tyrosine-
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



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